1,3-Dichlorotetrafluoroacetone

Other names:	2-Propanone, 1,3-dichloro-1,1,3,3-tetrafluoro- sym-Dichlorotetrafluoroacetone Bis(chlorodifluoromethyl) ketone DCTFA Stauffer N-3,412 1,1,3,3-Tetrafluoro-1,3-dichloroacetone 1,3-Dichloro-1,1,3,3-tetrafluoroacetone (CF2Cl)2CO Dichlorotetrafluoroacetone 1,3-Dichloro-1,1,3,3-tetrafluoro-2-propanone 4FK Acetone, 1,3-dichloro-1,1,3,3-tetrafluoroacetone NSC 62662
Inchi:	InChI=1S/C3Cl2F4O/c4-2(6,7)1(10)3(5,8)9
InchiKey:	QRKKTXWUDLJYCV-UHFFFAOYSA-N
Formula:	C3Cl2F4O
SMILES:	O=C(C(F)(F)Cl)C(F)(F)Cl
Mol. weight [g/mol]:	198.93
CAS:	127-21-9

Physical Properties

Property code	Value	Unit	Source
gf	-951.96	kJ/mol	Joback Method
hf	-1051.25	kJ/mol	Joback Method
hfus	11.01	kJ/mol	Joback Method
hvap	31.93	kJ/mol	Joback Method
ie	10.71 ± 0.01	eV	NIST Webbook
log10ws	-2.28		Crippen Method
logp	2.219		Crippen Method
mcvol	86.260	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	318.00 ± 4.00	K	NIST Webbook
tb	318.00	K	NIST Webbook
tb	317.70	K	NIST Webbook
tc	567.13	K	Joback Method
tf	240.54	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.73	J/mol×K	387.39	Joback Method
cpg	163.05	J/mol×K	417.35	Joback Method
cpg	168.80	J/mol×K	447.30	Joback Method
cpg	174.00	J/mol×K	477.26	Joback Method
cpg	178.69	J/mol×K	507.22	Joback Method
cpg	182.90	J/mol×K	537.17	Joback Method
cpg	186.66	J/mol×K	567.13	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C127219&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume